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Apr 8th, 9:00 AM - 10:00 AM

Diffusion and Aggregation of Metal Atoms on Quasicrystalline Surfaces

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Poster Presentation P67

**. DIFFUSION AND AGGREGATION OF METAL ATOMS ON
QUASICRYSTALLINE SURFACES**

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Quasicrystals are aperiodic structures with long-range orientational order. Unlike typical crystalline structures, quasicrystals do not have a unit cell, although similar groupings of atoms can be found repeatedly throughout the structure. Some quasicrystals exhibit interesting and potentially useful combinations of properties such as high heat conductivity, low coefficient of friction, and good wear resistance. The objective of this project was to investigate the interaction of metal atoms with a quasicrystalline surface, specifically the diffusion and aggregation of these atoms after deposition on the surface. The first part of the project focused on analyzing diffusion of silver atoms on an aluminum-palladium-manganese quasicrystal surface through computational techniques. Using a model potential energy surface for bonding of a silver atom to the quasicrystal, the relative positions of adsorption sites and activation barriers for hopping between them were determined. With this data, the effective diffusion coefficient was calculated at various temperatures. The second part of the project focused on describing by kinetic Monte Carlo simulation the diffusion and aggregation of aluminum atoms on an aluminum-copper-iron quasicrystal surface to compare with experimental observations.